

Singularities in fidelity surfaces for quantum phase transitions: a geometric perspective

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The fidelity per site between two ground states of a quantum lattice system corresponding to different values of the control parameter defines a surface embedded in a Euclidean space. The Gaussian curvature naturally quantifies quantum fluctuations that destroy orders at transition points. It turns out that quantum fluctuations wildly distort the fidelity surface near the transition points, at which the Gaussian curvature is singular in the thermodynamic limit. As a concrete example, the one-dimensional quantum Ising model in a transverse field is analyzed. We also perform a finite size scaling analysis for the transverse Ising model of finite sizes. The scaling behavior for the Gaussian curvature is numerically checked and the correlation length critical exponent is extracted, which is consistent with the conformal invariance at the critical point.

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Quantum phase transitions (QPTs) have been a research topic subject to intense study, since their significant role was realized in accounting for high- T_c superconductors, fractional quantum Hall liquids, and quantum magnets [1, 2]. Recently, significant advances have been made in attempt to clarify the connection between quantum many-body physics and quantum information science. This provides a new perspective to investigate QPTs from *entanglement* [3, 4, 5, 6, 7] and *fidelity* [8, 9, 10, 11, 12], basic notions of quantum information science [13] and turns out to be very insightful in our understanding of QPTs in a variety of quantum lattice systems in condensed matter.

Conventionally, orders and fluctuations provide a proper language to study QPTs, with order parameters being the key to quantify quantum fluctuations. Instead, the fidelity approach is based on state distinguishability arising from the orthogonality of different ground states in the thermodynamic limit. In fact, the ground state fidelity for a quantum system may be mapped onto the partition function of the equivalent classical statistical lattice model with the same geometry [11]. Thus, the fidelity per site is well-defined in the thermodynamic limit, and its singularities unveil transition points, at which the system under consideration undergoes QPTs. Therefore, a practical means is now available to map out the ground state phase diagram for a quantum lattice system without prior knowledge of order parameters. An intriguing question is how to characterize singularities in the fidelity per site. Indeed, a proper answer to this question will shed new light on our understanding of QPTs.

In this paper, we present an *intrinsic* characterization of singularities in the fidelity per site in terms of Riemannian geometry. For this purpose, we first *define* a fidelity surface as a surface embedded in a Euclidean space, which in turn is determined by the average fidelity per lattice site between two ground states of a quantum lattice system as a function of the control parameters. This makes the whole machinery developed in differential geometry of curves and surfaces available to study QPTs. As it is well known, the Gaussian curvature, or equivalently, the Ricci scalar curvature for the surfaces em-

bedded in Euclidean spaces, is a fundamental concept used to measure how curved a surface is. Therefore, the Gaussian curvature is expected to naturally quantifies quantum fluctuations that destroy orders at transition points. We discuss the global behaviors of the Gaussian curvature. It turns out that quantum fluctuations wildly distort the fidelity surfaces near the transition points. Generically, precursors of QPTs occur in the Gaussian curvature for finite-size systems. In the thermodynamic limit, the Gaussian curvature becomes singular at transition points. The one-dimensional quantum Ising model in a transverse field is exploited to explicitly illustrate the theory. We also perform a finite size scaling analysis for the Gaussian curvature with different lattice sizes to extract the correlation length critical exponent.

Fidelity surfaces. For a quantum lattice system described by a Hamiltonian $H(\lambda)$, with λ a control parameter. Here we restrict ourselves to discuss the simplest case with one single control parameter, although the extension to multiple control parameters is straightforward. For two ground states $|\psi(\lambda_1)\rangle$ and $|\psi(\lambda_2)\rangle$ corresponding to different values of the control parameter λ , the fidelity is defined as $F(\lambda_1, \lambda_2) \equiv |\langle\psi(\lambda_2)|\psi(\lambda_1)\rangle|$. For a large but finite L , the fidelity F asymptotically scales as $F(\lambda_1, \lambda_2) \sim d^L(\lambda_1, \lambda_2)$, where the scaling parameter $d(\lambda_1, \lambda_2)$ characterizes how fast the fidelity changes when the thermodynamic limit is approached [10]. Physically, it is the fidelity per site. Here note that the contribution from each site to $F(\lambda_1, \lambda_2)$ is multiplicative. Following [11], the ground state fidelity for a quantum system is nothing but the partition function of the equivalent classical statistical lattice model with the same geometry, if one utilizes the tensor network representations of ground state many-body wave functions. Therefore, $d(\lambda_1, \lambda_2)$ may be interpreted as the partition function per site [14], which is well-defined in the thermodynamic limit:

$$\ln d(\lambda_1, \lambda_2) = \lim_{L \rightarrow \infty} \ln F(\lambda_1, \lambda_2)/L. \quad (1)$$

The fidelity per site $d(\lambda_1, \lambda_2)$ satisfies the properties: (1) symmetry under interchange $\lambda_1 \longleftrightarrow \lambda_2$; (2) $d(\lambda_1, \lambda_1) = 1$; and (3) $0 \leq d(\lambda_1, \lambda_2) \leq 1$.

For simplicity, let us assume that the system undergoes a

QPT at λ_c . If $|\psi(\lambda_1)\rangle$ and $|\psi(\lambda_2)\rangle$ are in the same phase, then they flow to the same stable fixed point in the sense of renormalization group theory, and so their difference arises from quantum fluctuations depending on the details of the system. On the other hand, if $|\psi(\lambda_1)\rangle$ and $|\psi(\lambda_2)\rangle$ are in different phases, then they flow to two different stable fixed points. Therefore, they possess different orders, although quantum fluctuations originate from the same unstable fixed point λ_c [15]. Imagine that if there were no quantum fluctuations, then $d(\lambda_1, \lambda_2)$ would be simply 1 when $|\psi(\lambda_1)\rangle$ and $|\psi(\lambda_2)\rangle$ are in the same phase; otherwise, when $|\psi(\lambda_1)\rangle$ and $|\psi(\lambda_2)\rangle$ are in different phases, $d(\lambda_1, \lambda_2)$ would take the minimum value corresponding to the two stable fixed points. For continuous QPTs, quantum fluctuations are strong enough such that no orders survive at the transition point, so $d(\lambda_1, \lambda_2)$ is continuous, but displays singularities, whereas for the first order QPTs, $d(\lambda_1, \lambda_2)$ remains to be discontinuous at the transition point. An interesting observation is to regard the fidelity per site, $d(\lambda_1, \lambda_2)$, as a two-dimensional surface embedded in the three-dimensional Euclidean space, with a Riemannian metric induced from the Euclidean metric. Our aim is to give an *intrinsic* characterization of singularities in such a fidelity surface in terms of Riemannian geometry.

Differential geometry of the two-dimensional surfaces embedded in the three-dimensional Euclidean space. Let us briefly recall the fundamentals of differential geometry of surfaces embedded in Euclidean spaces [16]. For a two-dimensional surface embedded in a three-dimensional Euclidean space: $z = f(\lambda_1, \lambda_2)$, the first fundamental form on the surface is

$$dl^2 = g_{ij}d\lambda^i d\lambda^j = E(du)^2 + 2F(du dv) + G(dv)^2, \quad (2)$$

where g_{ij} is the Riemannian metric on the surface: $g_{11} = 1 + f_{\lambda_1}^2$, $g_{12} = g_{21} = f_{\lambda_1} f_{\lambda_2}$, and $g_{22} = 1 + f_{\lambda_2}^2$. Here the subscripts λ_1 and λ_2 denote partial differentiations with respect to λ_1 and λ_2 , respectively. In terms of the co-ordinates $u = \lambda_1$ and $v = \lambda_2$, we have $E = g_{11}$, $F = g_{12} = g_{21}$ and $G = g_{22}$. Suppose the surface is given in parametric form: $r = r(u, v)$. Then, the vector product $r_u \times r_v$ is a non-zero vector perpendicular to the surface at each non-singular point; define m to be a unit vector in the normal direction, then one has $r_u \times r_v = |r_u \times r_v|m$. For a curve $r = r(u(l), v(l))$ on the surface, the projection of the second order derivative \ddot{r} of r with respect to the arc length l on the normal to the surface leads to the second fundamental form as follows

$$\langle \ddot{r}, m \rangle (dl)^2 = b_{ij}d\lambda^i d\lambda^j = X(du)^2 + 2Y(du dv) + Z(dv)^2, \quad (3)$$

if a surface is given in the form $z = f(\lambda_1, \lambda_2)$ with $\lambda_1 = u$, $\lambda_2 = v$, and $r(u, v) = (u, v, f(u, v))$. Therefore, we have $X = b_{11} = f_{\lambda_1 \lambda_1} / \sqrt{1 + f_{\lambda_1}^2 + f_{\lambda_2}^2}$, $Y = b_{12} = b_{21} = f_{\lambda_1 \lambda_2} / \sqrt{1 + f_{\lambda_1}^2 + f_{\lambda_2}^2}$ and $Z = b_{22} = f_{\lambda_2 \lambda_2} / \sqrt{1 + f_{\lambda_1}^2 + f_{\lambda_2}^2}$.

The eigenvalues of the pair of quadratic forms (2) and (3) are the *principal curvatures* of the surface at the point under investigation. The product of the principal curvatures is the

Gaussian curvature K of the surface at the point, and their sum the *mean curvature*. The principal curvatures k_1 and k_2 are the solutions of equation:

$$\det(Q - kG) = 0, \quad (4)$$

where $Q = (b_{ij})$ is the matrix of the second fundamental form, and $G = (g_{ij})$. Since the first fundamental form is positive definite, its matrix G is non-singular. Hence $\det(Q - kG) = \det G \det(G^{-1}Q - k \cdot I)$, we deduce that the Gaussian curvature $K = k_1 k_2 = \det(G^{-1}Q) = \det Q / \det G$ and the mean curvature $M = k_1 + k_2 = \text{tr}(G^{-1}Q)$. Therefore, the Gaussian curvature K and the mean curvature M take the form:

$$K = \frac{f_{\lambda_1 \lambda_1} f_{\lambda_2 \lambda_2} - f_{\lambda_1 \lambda_2}^2}{(1 + f_{\lambda_1}^2 + f_{\lambda_2}^2)^2}, \quad (5)$$

and

$$M = \frac{(1 + f_{\lambda_2}^2)f_{\lambda_1 \lambda_1} + (1 + f_{\lambda_1}^2)f_{\lambda_2 \lambda_2} - 2f_{\lambda_1} f_{\lambda_2} f_{\lambda_1 \lambda_2}}{(1 + f_{\lambda_1}^2 + f_{\lambda_2}^2)^{3/2}}, \quad (6)$$

respectively. We notice that the sign of the *Gaussian curvature* K is the same as the sign of the determinant: $f_{\lambda_1 \lambda_1} f_{\lambda_2 \lambda_2} - f_{\lambda_1 \lambda_2}^2$, i.e., the *Hessian* of $z = f(\lambda_1, \lambda_2)$

It follows that, in contrast with the mean curvature M , the Gaussian curvature K of a surface may be expressed in terms of the induced metric on the surface alone, and is therefore an intrinsic invariant of the surface [16]. In addition, a two-dimensional surface in a three-dimensional space may also be regarded as a differentiable manifold endowed with a Riemannian metric induced from the Euclidean metric. The Ricci scalar curvature R is twice the Gaussian curvature K : $R = 2K$.

Global behaviors of the Gaussian curvature K for a fidelity surface. Now we consider the (logarithmic function of) fidelity per site, $\ln d(\lambda_1, \lambda_2)$, as a two-dimensional surface embedded in the three-dimensional Euclidean space: $z = f(\lambda_1, \lambda_2) \equiv \ln d(\lambda_1, \lambda_2)$. The Gaussian curvature $K(\lambda_1, \lambda_2)$ for such a fidelity surface may be used to quantify how strong quantum fluctuations are in given quantum many-body ground states, thus providing an intrinsic characterization of singularities in the fidelity surface. Indeed, as justified in Refs. [9, 10, 11], the fidelity per site $d(\lambda_1, \lambda_2)$ is singular when $\lambda_1(\lambda_2)$ crosses λ_c for a fixed $\lambda_2(\lambda_1)$ in the thermodynamic limit. Therefore the Gaussian curvature $K(\lambda_1, \lambda_2)$ for the fidelity surface is singular at $\lambda_1 = \lambda_c$ and/or $\lambda_2 = \lambda_c$ in the thermodynamic limit. Generically, we have: (1) $K(\lambda_1, \lambda_2) > 0$, there is a neighborhood of the point throughout which the surface lies on one sides of the tangent plane at the points; (2) $K(\lambda_1, \lambda_2) < 0$, then the surface intersects the tangent plane at the point arbitrarily close to the point. If the surface is strictly convex, then we say that the Gaussian curvature $K(\lambda_1, \lambda_2)$ is positive at every point of the surface. That is what happens if λ_1 and λ_2 are away from the transition point. However, if λ_1 and λ_2 are close to the transition point, then the Gaussian curvature $K(\lambda_1, \lambda_2)$ can be negative.

For finite-size systems, the Gaussian curvature $K(\lambda_1, \lambda_2)$ remains to be smooth, although the precursors of QPTs occur as anomalies in the Gaussian curvature $K(\lambda_1, \lambda_2)$. The anomalies get more pronounced when the thermodynamic limit is approached. We may take advantage of this fact to perform finite size scaling to extract the correlation length critical exponent.

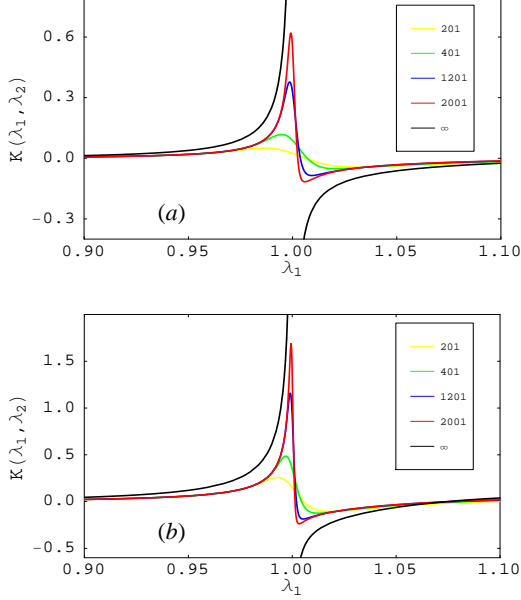


FIG. 1: (color online) The behavior near the critical point $\lambda_c = 1$ is analyzed for the Gaussian curvature $K(\lambda_1, \lambda_2)$ of the quantum transverse Ising model for various lattice sizes. The curves shown correspond to different lattice sizes $L = 201, 401, 1201, 2001$, and ∞ . The peaks (dips) get more pronounced in the left (right) side with increasing system size. The Gaussian curvature $K(\lambda_1, \lambda_2)$ diverges at the critical point $\lambda_1 = \lambda_c$ for the infinite-size system ($L = \infty$). Upper panel: Here $K(\lambda_1, \lambda_2)$ is regarded as a function of λ_1 for $\lambda_2 = 0.6$ and $\gamma = 1$. Lower panel: Here $K(\lambda_1, \lambda_2)$ is regarded as a function of λ_1 for $\lambda_2 = 0.6$ and $\gamma = 1/2$.

Quantum XY spin 1/2 model. The quantum XY spin model is described by the Hamiltonian

$$H = - \sum_{j=-M}^M \left(\frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y + \lambda \sigma_j^z \right). \quad (7)$$

Here σ_j^x, σ_j^y and σ_j^z are the Pauli matrices at the j -th lattice site. The parameter γ denotes an anisotropy in the nearest-neighbor spin-spin interaction, whereas λ is an external magnetic field. The Hamiltonian (7) may be exactly diagonalized [17, 18] for any finite size L with $L = 2M + 1$. In the thermodynamic limit $L \rightarrow \infty$, $\ln d(\lambda_1, \lambda_2)$ takes the form [9]:

$$\ln d(\lambda_1, \lambda_2) = \frac{1}{2\pi} \int_0^\pi d\alpha \ln \mathcal{F}(\lambda_1, \lambda_2; \alpha), \quad (8)$$

where $\mathcal{F}(\lambda_1, \lambda_2; \alpha) = \cos[\vartheta(\lambda_1; \alpha) - \vartheta(\lambda_2; \alpha)]/2$, with $\cos \vartheta(\lambda; \alpha) = (\cos \alpha - \lambda) / \sqrt{(\cos \alpha - \lambda)^2 + \gamma^2 \sin^2 \alpha}$ [19].

Now it is straightforward to calculate the Gaussian curvature $K(\lambda_1, \lambda_2)$ for the fidelity surface of the quantum XY spin chain. In Fig. 1, we plot $K(\lambda_1, \lambda_2 = 0.6)$ for the fidelity surface of the quantum XY model ($\gamma = 1$ for the upper panel and $\gamma = 1/2$ for the lower panel). One observes that $K(\lambda_1, \lambda_2 = 0.6)$ is divergent as a function of λ_1 at the critical point $\lambda_c = 1$ for the infinite-size system $L = \infty$, indicating that the fidelity surface is wildly distorted, due to strong quantum fluctuations near the critical point. This is true for any nonzero γ , consistent with the fact that the quantum XY model for any nonzero γ belongs to the same universality class as the quantum transverse Ising model. That is, there is a critical line $\gamma \neq 0$ and $\lambda_c = 1$; only one (second-order) critical point $\lambda_c = 1$ separates two gapful phases: (spin reversal) Z_2 symmetry-breaking and symmetric phases.

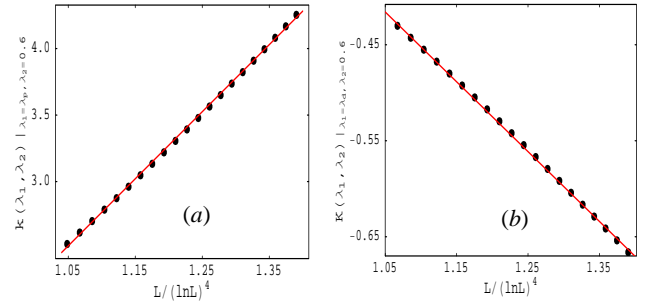


FIG. 2: (color online) (a) The peaks values of the Gaussian curvature $K(\lambda_1, \lambda_2)$ of the quantum transverse Ising model for large lattice sizes scale as $L/(\ln L)^4$. (b) The dips values of the Gaussian curvature $K(\lambda_1, \lambda_2)$ of the quantum transverse Ising model for large lattice sizes scale as $L/(\ln L)^4$. In both cases, $\lambda_2 = 0.6$ and $\gamma = 1$.

Finite size scaling analysis for the Gaussian curvature K .

We focus on the quantum Ising universality class. The order parameter, i.e., magnetization $\langle \sigma^x \rangle$ is non-zero for $\lambda < 1$, and otherwise zero. At the critical point, the correlation length $\xi \sim |\lambda - \lambda_c|^{-\nu}$ with $\nu = 1$ [18]. In order to analyze how the Gaussian curvature $K(\lambda_1, \lambda_2)$ behaves near the critical point $\lambda_c = 1$, we perform a finite size scaling analysis for the quantum transverse Ising model.

As already observed, the drastic change of the ground state wave functions makes the Gaussian curvature $K(\lambda_1, \lambda_2)$ divergent when the system undergoes the second order QPT at the critical point $\lambda_c = 1$ in the thermodynamic limit. However, for finite-size systems, $K(\lambda_1, \lambda_2)$ remains to be smooth for the quantum XY model. In Fig. 1, the numerical results are also plotted for the Gaussian curvature $K(\lambda_1, \lambda_2)$ with different system sizes, where $\lambda_2 = 0.6$ and $\gamma = 1$ (upper panel) and $\lambda_2 = 0.6$ and $\gamma = 1/2$ (lower panel). More precisely, in the thermodynamic limit, $K(\lambda_1, \lambda_2)$ (as a function of λ_1 for a fixed λ_2) diverges at the critical point $\lambda_1 = \lambda_c$:

$$K(\lambda_1, \lambda_2) \sim \frac{1}{|\lambda_1 - \lambda_c| (\ln |\lambda_1 - \lambda_c|)^4}. \quad (9)$$

However, there is no divergence for finite-size systems, but there are clear anomalies, featuring two quasi-critical values

λ_p and λ_d , one at each side of the critical point. On the left (right) side, the so-called quasi-critical points λ_p (λ_d) approach the critical value as $\lambda_p \approx 1 - 1.6149L^{-1.03531}$ ($\lambda_d \approx 1 + 9.69198L^{-0.974152}$), with the values at peaks (dips) diverging with increasing system size L :

$$K(\lambda_1, \lambda_2)|_{\lambda_1=\lambda_{p(d)}} = k_{p(d)} \frac{L}{(\ln L)^4} + \text{constant}. \quad (10)$$

Here the prefactor $k_{p(d)}$ is non-universal in the sense that it depends on λ_2 and γ . We emphasize that Eq. (10) follows from Eq. (9), if we take into account the fact that the model is conformally invariant at the critical point. Indeed, on the one hand, from Eq. (9) and the correlation length $\xi \sim |\lambda - \lambda_c|^{-\nu}$ with $\nu = 1$, we have $K(\lambda_1, \lambda_2) \sim \xi/(\ln \xi)^4$. On the other hand, the conformal invariance requires the scale invariance: $\xi/L = \xi'/L'$. The numerical results are, respectively, plotted for $K(\lambda_1, \lambda_2)|_{\lambda_1=\lambda_{p(d)}}$ in Fig. 2 and for $\lambda_{p(d)}$ in Fig. 3 with $\lambda_2 = 0.6$ and $\gamma = 1$. The same is also true for any nonzero γ . This shows that, consistent with the exact result, the correlation length critical exponent ν equals 1, as long as γ is nonzero.

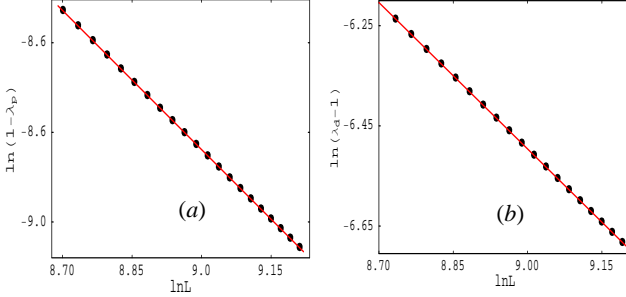


FIG. 3: (color online) (a): The positions of the peaks approach the critical point $\lambda_c = 1$ with increasing system size L as $\lambda_p \approx 1 - 1.61490L^{-1.03531}$. (b) The positions of the dips approach the critical point $\lambda_c = 1$ with increasing system size L as $\lambda_d \approx 1 + 9.69198L^{-0.974152}$. In both cases, $\lambda_2 = 0.6$ and $\gamma = 1$.

Conclusions. We have shown that singularities in fidelity surfaces may be *intrinsically* characterized in terms of Riemannian geometry, based on the fidelity description of QPTs. Generically, the Ricci curvature tensor for finite-size systems is analytic and it exhibits singularities at transition points in the thermodynamic limit, as reflected in the Ricci scalar curvature that blows up when the system size tends to ∞ . This opens up the possibility to exploit the theory of Ricci flows [20] to characterize QPTs in condensed matter theory. The one-dimensional quantum Ising model in a transverse field is exploited as an example to explicitly illustrate the theory [21], and a finite size scaling analysis has been performed for the Ricci scalar curvature with different lattice sizes, and the correlation length critical exponent has been extracted, consistent with the known exact value.

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